United States
Environmental Protection
Agency

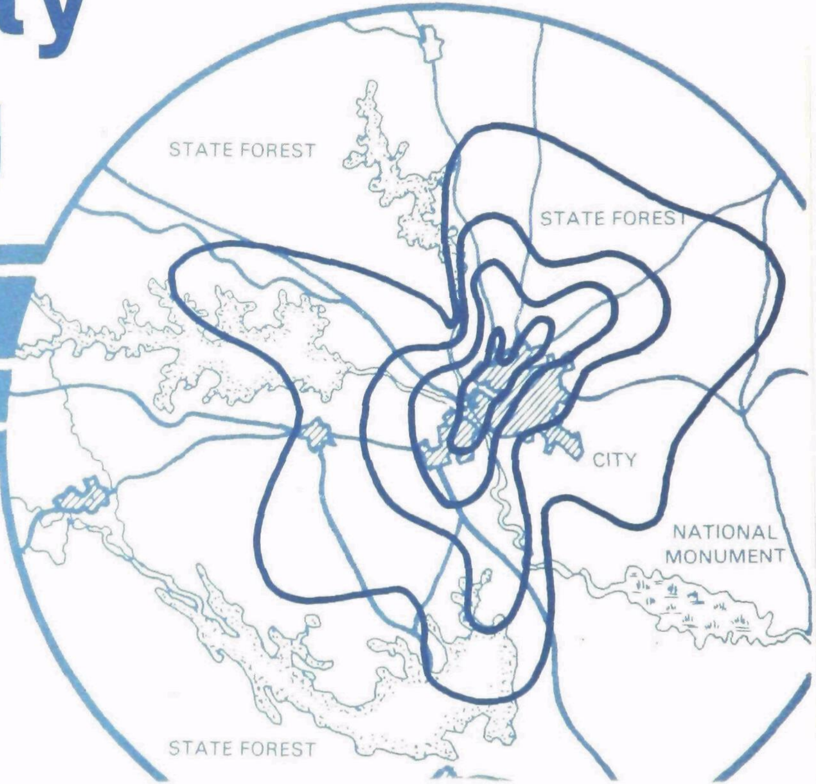
Office of Air Quality
Planning and Standards
Research Triangle Park, NC 27711

September 1980

Air

Air Quality Modeling

What It Is and How It Is Used



This publication was prepared for the U.S. Environmental Protection Agency under contract by Environmental Research & Technology, Inc., Concord, MA. Among many individuals who contributed to the brochure in the review process, the efforts of Carol Counihan and Dr. Bruce Egan are especially appreciated.

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EPA is charged by Congress to protect the Nation's land, air and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise and radiation, the Agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

Foreword

The purpose of this brochure is to acquaint the reader with the basic concepts of air quality modeling and its application in air quality management. It is directed to non-technical audiences to explain what models are, how they are used, and what their limitations are as a tool in the air pollution control process. Several publications are listed for those who desire further information.

It should be understood that models are mathematically derived tools. The reliability of predicted air quality estimates is directly dependent upon the detail and quality of the information used in applying the models. Their primary purpose is to serve as an aid in arriving at sound regulatory decisions.

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Glossary of Terms

Area Source: a group of pollutant emitting facilities, with small and variable emission rates, which are evenly distributed across a well-defined region. Emissions from residential and commercial space heating furnaces over several city blocks may be modeled as one area source.

Background Pollutant Concentration: that portion of observed ambient pollutant concentrations which is not directly attributable to major nearby pollutant sources.

Chemical Removal Process: a series of chemical reactions which changes the chemical composition of a pollutant. Such transformations reduce the amount of the original pollutant in the ambient atmosphere.

Dispersion/Diffusion: a mixing process in which air motions mix a pollutant plume over an ever increasing volume, thereby diluting the concentration of the pollutant in the ambient air.

Line Source: a pollutant producing activity which is uniformly spread out along a narrow band. Pollutant emissions from moving vehicles on a major highway may be modeled as a line source.

Long-Term: a period of time associated with annual air quality standards. Long-term models usually address pollutant concentrations over several seasons to one year.

Meteorological Episode or Event: a short period of time, varying between one hour and a few days, over which a single class of weather conditions is dominant.

Physical Removal Process: a series of events which leads to the direct depletion of an air pollutant in the ambient atmosphere without chemical transformation. Several physical mechanisms include settling of heavy particles, impaction on vegetation and structures, and rainout.

Point Source: a single activity that causes the release of a pollutant plume from a stationary vent. Large smokestack emissions are modeled as a single point source.

Primary Pollutant: a substance which is produced by a source and released directly into the atmosphere as a pollutant.

Secondary Pollutant: a pollutant which forms in the atmosphere as a result of chemical reactions between substances released by a source, and other substances already present in the atmosphere. Many of these reactions depend on sunlight, and are called photochemical reactions.

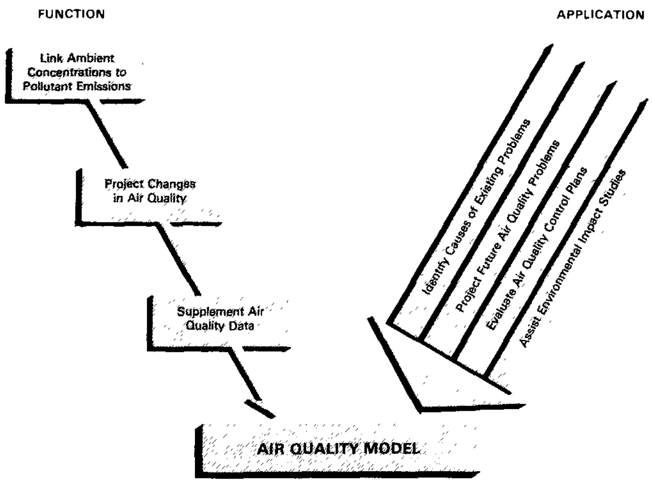
Short-Term: a period of time associated with air quality standards for pollutant exposures ranging between one hour and 24 hours.

"Worst-Case" Meteorology: a specific combination of wind speed, wind direction, and other weather variables which fosters the highest expected pollutant concentrations due to emissions from a particular group of air pollution sources.

Air Quality Modeling in Decision-Making

What is an air quality model?

An air quality model is a set of mathematical equations relating the release of air pollutants to the corresponding concentrations of pollutants in the ambient atmosphere. Ambient air is the outdoor air to which people, structures, plants, and animals are exposed. Such mathematical relationships provide a technique for predicting the consequences of changing the amount of pollutants released into the air from either new or existing sources of air pollutants.



What are air quality models used for?

Air quality models are used to identify and evaluate the level of controls required to solve industrial and urban air pollution problems. They are applied in an engineering or analytical way to identify the causes of existing problems, and in a planning or predictive way to project and avoid future problems. Air quality models are used to:

- develop air pollution control plans for attainment and maintenance of acceptable air quality,
- assess environmental impacts expected from industrial expansion and urban development, and
- project the future air quality trends and patterns associated with regional planning options.

Each of these model applications is illustrated by an example.

- Unacceptably high ambient pollutant concentrations are measured in a residential area near an industrial zone containing many large pollutant sources. Modeling must be used to identify which sources are contributing to the excessive concentrations. Once the problem sources are identified, air quality engineers can take appropriate action to solve the problem. By administrative action the state agency can then incorporate this solution into the state air pollution control plan.
- An industry wants to construct a major new facility in an industrial park near a large urban area and submits an application to the state for a permit to construct. Modeling must be used by the state agency or industrial consultants to predict how emissions from the new facility will affect ambient air quality. The state and federal air pollution authorities will issue a permit to construct only if the modeling indicates that acceptable air quality will be maintained after the facility is in operation.
- A regional planning agency has several different options for industrial expansion in a rural county. Based on typical source characteristics and projected emissions, the impact of each option can be assessed with an appropriate air quality model. The model results can be used in conjunction with other information to rank each option. In this way environmental and economic factors can be clearly assessed and integrated in the planning process.

In each case, modeling provides a quantitative link between sources of air pollutants and ambient air quality. Such a link is necessary when regulatory decisions must be made within the framework of the air quality standards and Prevention of Significant Deterioration (PSD) increments.

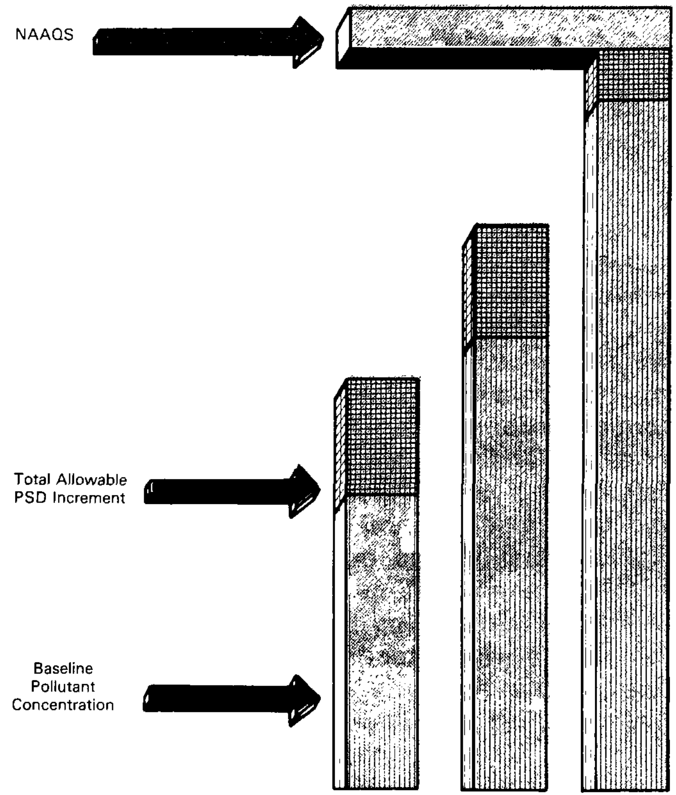
What are the air quality standards and PSD increments?

National Ambient Air Quality Standards (NAAQS) are maximum pollutant concentration limits for ambient air in the United States. The U.S. Environmental Protection Agency (EPA) and state air pollution agencies must ensure that NAAQS are attained and maintained throughout the country.

Primary NAAQS protect the public health and are based on known health effects. Secondary NAAQS are generally more restrictive than primary standards. They are based on vegetative and material effects and are intended to protect public welfare.

The PSD program was established to maintain the ambient air quality existing on a specific baseline date. The program applies, on a pollutant-specific basis, to areas of the country where existing air pollutant concentrations are below the limits specified by NAAQS.

PSD increments are ambient pollutant concentration limits which legally define how much pollutant concentrations in an area can increase from a set baseline level for all future time. As new pollutant sources come on-line and each increases ambient pollutant concentrations slightly, they are said to "consume available increment." The full increment is available to these



sources if the difference between the NAAQS and the baseline level is greater than the increment.

When are models used to assess compliance with the standards and PSD increments?

Compliance with the ambient air quality standards is primarily assessed with ambient air quality monitoring data, when that data exist. However, the geographical coverage and sampling frequency achievable in most monitoring systems limits the ability of the system to document all possible occurrences of high pollutant concentrations. Consequently, supplemental modeling analyses are frequently performed to determine if the standards are being attained and maintained in areas where it is suspected that air quality data do not include maximum possible concentrations.

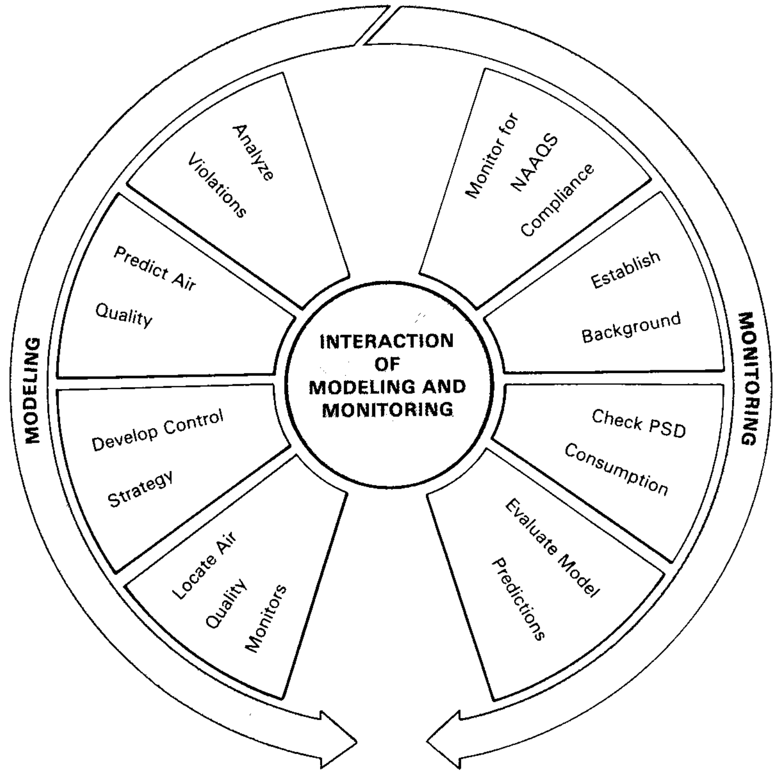
Air quality modeling becomes essential when compliance with standards must be assessed during permit review for new major sources. The analysis must evaluate whether or not allowed emissions from the new source will cause or contribute to a violation of a NAAQS.

The consumption and allocation of PSD increments is also calculated with modeling. This is because PSD permit conditions demand that increment consumption expected from new major sources and major modifications of existing sources be predicted in advance of granting the permit.

What is the relationship between monitoring and modeling?

Collection and analysis of air quality data is useful in (1) providing model validation data, (2) monitoring for NAAQS attainment and maintenance, and (3) establishing background pollutant concentrations due to minor or distant sources not included in dispersion calculations. In cases where there are few existing sources in the area of a proposed new source or modification, monitoring may also provide a check on the maintenance of applicable PSD increments. Each of these functions is directly related to the use of models.

Ambient air quality monitoring ultimately determines the validity of modeling assumptions. The most valuable interaction between monitoring and modeling occurs when modeling is used to identify areas of highest expected pollutant concentrations, and subsequent monitoring near these locations is used to evaluate model predictions, and to ensure that air quality standards are maintained. A second type of interaction frequently occurs when monitors record excursions of the standards. Such excursions usually trigger modeling analyses to develop a control strategy aimed at correcting the causes of the violations. In both cases, modeling is used as a predictive tool in identifying which sources have an important air quality impact and where these impacts occur, while monitoring provides a basis for assessing the accuracy of those predictions.



Applying Air Quality Models

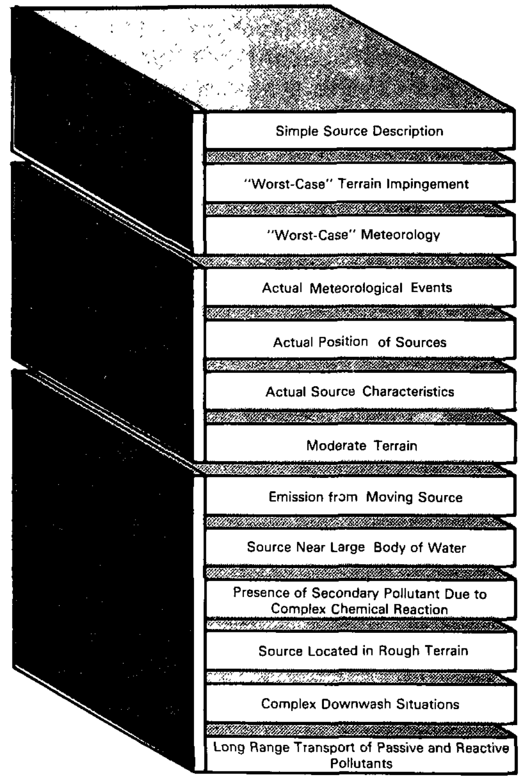
What is the general approach to modeling?

Generally accepted practice calls for a two step modeling procedure. The first step provides for a screening of potential air quality problems with the use of a simple model. The second step is a detailed assessment of an air quality problem identified in the screening analysis, using a more refined model. The second step is initiated if potential air quality problems, such as violations of NAAQS, are singled out in the first step.

What is a screening analysis?

The purpose of a screening analysis is to eliminate, with minimum effort, those sources that clearly will not cause or contribute to ambient concentrations in excess of any air quality standard. When properly applied, screening models can eliminate unnecessary expenditures of resources associated with more refined modeling assessments.

The screening procedure is most useful for point sources when the short-term standards are more limiting than long-term standards. The first



phase of the procedure consists of simple calculations for estimating concentrations under worst-case meteorological situations not complicated by terrain or other physical features. A second phase includes more detailed screening procedures for special cases including simple terrain impingement, building downwash, and long range transport.

What is a refined model analysis?

A refined model incorporates many of the same assumptions found in the more complex screening models. However, the refined model retains much more of the detail present in source data and meteorological data. While screening model predictions consider worst-case meteorological conditions and simplified physical assumptions, the refined model incorporates more complex physical assumptions, and uses the actual distribution of meteorological episodes and source characteristics to assess the potential for ambient air quality violations.

What kinds of data are needed to apply a model?

Data needed to apply a model fall into three categories:

- source data
- air quality data
- meteorological data

Source data describe where pollutants are released, and determine initial pollutant concentrations. Air quality data provide information on background pollutant concentrations that either add to or react with pollutants included in the source data. Meteorological data describe the potential for pollutant transport, diffusion, and transformation in the atmosphere before reaching the ground.

What source information is needed?

All simulation models require at least the following source information:

- location of air pollution sources

- estimates of the amount of pollutant that each can emit
- description of how pollutants are released to the atmosphere
- description of nearby structures

The location of a source of air pollution is usually referenced to a conventional map coordinate system. This enables a model to specify the individual locations of each source relative to significant terrain features, populated areas, other sources, and air quality monitors. A description of the pollutant-producing process at each source is used to estimate the amount of pollutants emitted to the atmosphere, and a description of how the pollutants are emitted determines what atmospheric processes are important in estimating ambient concentrations resulting from these emissions.

All of this information is generally obtained from engineering, process, and fuel use data. The specific quantities derived from this data and used to model each source include:

- source coordinates,
- pollutant emission rate
- height of the pollutant release such as stack or vent height
- shape and dimensions of release points such as the stack diameter of a point source, or the width and length of an area source
- temperature of the plume upon release to the atmosphere
- velocity of plume at the point of atmospheric release
- dimensions and locations of nearby buildings and structures

Source information is generally obtained from local and state air pollution agencies, and the EPA. Each EPA regional office collects and maintains emissions data, and makes it available to the general public. State agencies submit detailed source data to these offices annually. Therefore, local and state agencies often provide detailed source data directly from their own emissions inventory system. Regional emissions over the entire country can be found in the National

Emissions Data System (NEDS), which is maintained by the EPA.

What air quality information is needed?

Air quality data from existing monitoring stations is needed to provide information on ambient pollutant concentrations. When obtained from appropriate monitors, these data are used to determine if an area is in compliance with NAAQS, and are also used to adjust air quality model estimates for background pollutant concentrations. These data can be obtained from state and local air pollution control agencies, or through the **S**torage **A**nd **R**etrieval **O**f **A**erometric **D**ata (SAROAD) system at regional EPA offices. The SAROAD system is the national air data bank. These sources may be supplemented with data from industrial monitoring networks. Most measurements are processed into short-term and annual averages for convenient comparison with NAAQS.

What meteorological information is needed?

Meteorological variables that describe pollutant transport and dispersion in the atmosphere are wind direction, wind speed, atmospheric stability, and mixing height. Wind direction determines the general direction of pollutant transport. Wind speed determines the amount of initial dilution of the pollutants and also the height to which the plume rises. Atmospheric stability is a measure of turbulence, which in turn determines the rate at which the effluent is dispersed as it is transported by the wind. Mixing height is the vertical depth of the atmosphere through which pollutants can be dispersed.

Estimates of each variable are usually obtained from meteorological observations made by the National Weather Service (NWS) at numerous observing stations throughout the country. They are available as hour-by-hour weather observations and in summarized forms from the National Climatic Center (NCC) in Asheville, North Carolina. The variables can also be obtained from similar information recorded by industrial site-specific meteorological measurement programs.

Other variables, such as relative humidity and solar radiation, may be required for sophisticated air quality models that simulate chemical reactions and transformations in the atmosphere. These variables can be inferred through appropriate analysis of NWS data and site-specific measurements.

What determines the selection of a particular model?

The choice of a model depends primarily on the level of detail required to fulfill the objectives of the analysis, on the availability of input data, and on the physical nature of the system to be analyzed.

Analysis objectives can include siting air quality monitors, or assessing compliance with air quality standards, for example. In siting monitors, zones of high, frequently occurring concentrations must be identified. When compliance modeling is performed, only the highest, or second highest predicted concentrations are of interest. Modeling approaches in those two cases may not be the same.

The availability of input data can influence the selection of an air quality model. The more complex models generally require more detailed data bases. However, the availability of this information alone does not control the choice of model. In some cases, limited use of representative data to augment existing data required for a more complex model will produce considerably more useful and accurate concentration estimates than those produced by a less complex model that happens to fit the existing data.

The physical nature of the system depends on (1) the characteristics of the pollutants, (2) the averaging time for determining pollutant concentrations, (3) the characteristics of the sources of those pollutants, and (4) the characteristics of transport and diffusion between those sources and points selected for air quality evaluation. Elements of these four factors are listed in Table 1.

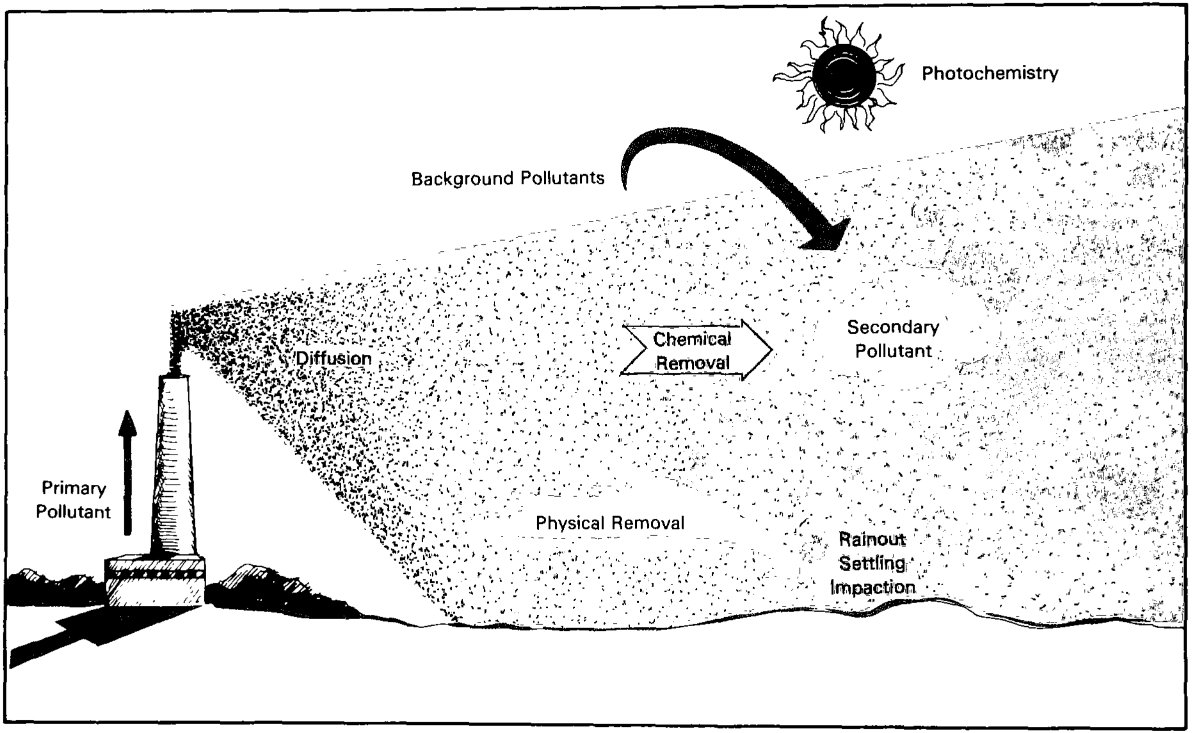
What computer resources are required?

The simplest screening calculations can be done with no more than a scientific pocket calculator. However, more complicated analyses are performed with a small computer.

Table 1
Factors Important in Selecting a Model

Pollutant Characteristics	
Production Process	**Removal Process**
1. Primary	1. None
2. Secondary	2. Chemical
	3. Physical
Averaging Time	
Short-term	**Long-term**
1. Hours	1. Months
2. Days	2. Seasons
Source Characteristics	
Number	**Geometry**
1. Few/Isolated	1. Point
2. Multiple	2. Area
	3. Line
	4. Volume
Transport and Diffusion Characteristics	
Geographic Features	**Distance**
1. Simple	1. Short-range ($\leq$ 50 km)
2. Complex	2. Long-range (>50 km)

All refined models require a large computer. The capabilities of a large computer are needed since many meteorological conditions must be simulated, and concentrations at many receptor locations must be calculated for each meteorological condition.



Pollutant characteristics and transport characteristics are important factors in selecting a model. Some pollutants (primary) are nearly inert over short-range downwind distances, and their concentration in the atmosphere only changes through diffusion. Over long-range downwind distances, these pollutants eventually leave the atmosphere mainly through physical removal processes. Other primary pollutants are chemically reactive. They can be removed through chemical transformations. Pollutants created by these chemical reactions are called secondary pollutants.

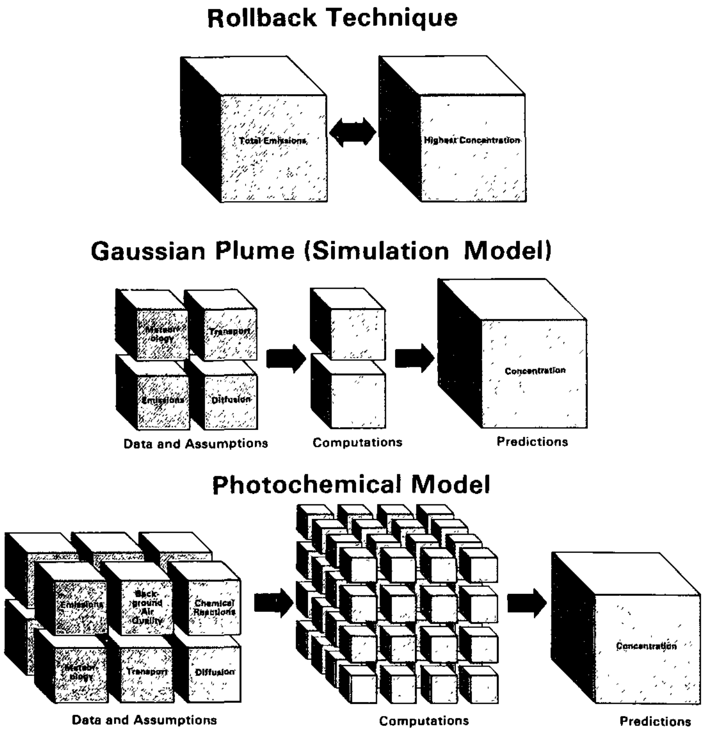
Available Air Quality Models

What are the general types of air quality models?

There are a number of different types of models ranging from quite simple to complex. The simplest type of air quality model is the proportional "rollback" technique which is useful if very little information is known, and crude estimates of needed emissions reductions are desired. The technique assumes that changes in the highest concentrations of a particular pollutant are directly related to the changes in the areawide emissions of that pollutant. Using this technique, a required 50% reduction in ambient concentrations needs a 50% reduction (or rollback) in regional emissions. In contrast, one of the most complicated forms of an air quality model is a photochemical model for reactive pollutants. This type of model can contain many complicated chemical reaction relationships which require a vast number of computations. Extensive and detailed emissions, air quality, and meteorological data must be available in order to apply this type of model.

Between these two extremes lies a variety of statistical and simulation models. Statistical models are similar to the rollback techniques, relying on observed relationships between air quality data, emission rates, and selected meteorological variables. These models are site-specific. Simulation models, on the other hand, explicitly incorporate the effects of physical and chemical processes through mathematical expressions derived from fundamental scientific principles. As a result, the same simulation model can be conveniently and correctly applied in many different regions as long as the basic model assumptions are not violated. This is not true of statistical models. Therefore, most air quality modeling is performed with simulation models.

The most frequently used screening and refined simulation models for evaluating the dispersion of atmospheric contaminants are those based on the well-known Gaussian plume description of the dispersion process. Gaussian plume models simulate transport and diffusion of air pollutants by means of simple algebraic expressions that are easily programmed for a computer. These models have been used for more than two decades, and



underlie much of the current and proposed regulatory modeling practice. They will continue to be widely used in the future. Nearly all available atmospheric dispersion models are based on the Gaussian description.

What is the EPA UNAMAP series?

The **U**ser's **N**etwork for **A**pplied **M**odels of **A**ir **P**ollution (UNAMAP), instituted in 1973 by the EPA, is a system consisting of a library of air quality simulation models. EPA stores the models for readily available access, updates the models and model inventory, and provides a service that notifies users of any changes to the models. The UNAMAP series includes both screening models and refined models and is available on magnetic tape from the National Technical Information Service (NTIS).

What models are included in UNAMAP?

The UNAMAP models, listed in Table 2, are all Gaussian-based dispersion models. Gaussian models have been used extensively in atmospheric dispersion modeling and form the basis for much of the current regulatory procedures.

Table 2
Summary of Models in UNAMAP

- APRAC, a short-term model for vehicle-generated pollutants located within and around an urban area.
- HIWAY, a short-term model for vehicle-generated pollutants for calculating concentrations downwind of roadways.
- PTMAX, PTDIS, short-term screening models for a single source in rural areas. These models determine distances of maximum concentrations for specific meteorological conditions.
- PTMTP, a short-term screening model for multiple sources in rural areas.
- PAL, a point, area, and line source screening model for calculating short-term concentrations in rural areas.
- CDM, **C**limatological **D**ispersion **M**odel, an annual or seasonal urban model.
- CDMQC, version of CDM capable of identifying individual source contributions to the predicted pollutant concentrations.
- RAM, a series of models for calculating short-term and annual concentrations during a one-year period in flat urban areas with point and area sources in multiple locations.
- CRSTER, a model for calculating short-term and annual concentrations during a one-year period from a single plant in a rural area with moderate terrain.
- VALLEY, a screening model for calculating maximum 24-hour concentrations from a single source in rural rough terrain.
- ISC, a model for estimating short-term and annual concentrations during a one-year period for complex industrial sources.
- MPTER, a model for estimating short-term and annual concentrations during a one-year period from multiple sources in a rural area with moderate terrain.

UNAMAP models incorporate a wide variety of features and capabilities. Most of the models handle primary pollutants without any consideration for physical or chemical removal processes. None handle the secondary production process directly, while several approximate physical and chemical removal processes with a simple mathematical formulation. A majority of the models can be applied to estimate short-term concentrations while about half can be used for longer averaging periods.

When may other models be used?

When circumstances become sufficiently complicated, other refined models may be required. Such models, when available, should be applied cautiously and only under the direction of experienced air pollution engineers or scientists. They can be used to assess:

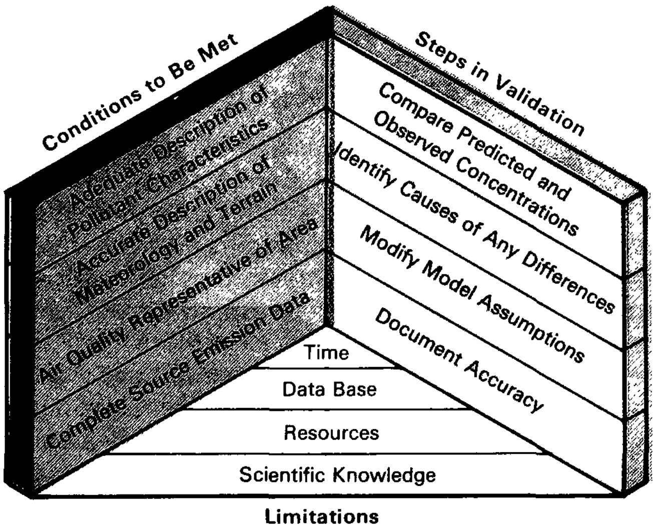
- emission releases from sources located in areas with rough or complex terrain
- emission releases from sources near large bodies of water
- the formation of secondary pollutants through complex chemical reactions
- the long-range transport of both passive and reactive pollutants
- emissions from moving sources such as jet aircraft
- complicated downwashing situations which are beyond the limitations of the ISC UNAMAP model

Accuracy of Air Quality Modeling, and Decision-Making

What determines the adequacy of a model?

A model is considered adequate if it predicts observed pollutant concentrations well. This usually occurs when the model incorporates all of the important physical processes which determine maximum pollutant concentrations.

For example, plumes from short, stubby stacks close to large buildings are known to downwash at high wind speeds. (A plume caught in disturbed air flow patterns in the wake of a structure reaches the ground quickly and is said to "downwash.") If a model for such a plume does not include this process, it will fail to produce adequate predictions of pollutant concentrations close to the stack.



Modeling adequacy is more difficult to assess in complex situations. The physical processes which are most important may not be clear. If model adequacy is in doubt, validation or calibration studies are required to test the ability of the model to predict observed concentrations.

How is a model validated?

A model can be validated if its predictions are directly comparable to detailed air quality observations. When comparisons are made, the following conditions must be met:

- Terrain and meteorological conditions are described adequately in the model.
- Source data are complete and any significant variations are identified.

- Pollutant characteristics are well known, including any important chemical reactions or removal processes.
- The pollutants to be addressed must have characteristics similar to those for which the model was developed.
- Air quality data are representative of the area and averaging times simulated, and are accurate and complete.

When these conditions are satisfied, validation of the model consists of the following steps:

- Simulated concentrations are compared with measured data.
- The causes of any differences are identified.
- Data bases are corrected and improved.
- Inappropriate model assumptions are modified.
- The accuracy of predicted concentrations is documented.

If a statistical evaluation of the results of comparing predicted and observed concentrations indicates that predicted concentrations do not compare well with measured concentrations, then it is likely that one or both of the following problems exist: (1) the source data, meteorological data, or air quality data are not appropriate, reliable, and complete or (2) the model itself is inadequate. Due to limitations in data bases, scientific knowledge, time, and resources, a complete validation is not always possible.

What is the expected accuracy of models?

Realistic assumptions used in air quality models are in accordance with experience and scientific theory, but they are at best only approximations. When coupled with the inaccuracies inherent in the source data and the meteorological data used in the model, use of these approximations will sometimes cause a model to either overpredict or underpredict short-term concentrations. When specific meteorological events are considered, model predictions are generally within a factor of 2 of the observed concentrations.

How should air quality data be used to verify model-based decisions?

Air quality data are used to verify model-based decisions in a broad sense by indicating if the NAAQS are maintained, or if further progress is made toward attaining the standards in non-attainment areas. In a more specific sense, air quality data may also be used to test the applicability of the modeling, and thereby either lend support to the predictions of the model, or provide a basis for re-evaluating the modeling assumptions employed.

If a detailed emissions and meteorological data base is collected in conjunction with monitored air quality data, then a comparison of model predictions, using actual emission rates, with the observed pollutant concentrations is possible. Such a comparison may lead to a recommendation for the use of an alternate model. When it is evident that the model consistently under-predicts the highest of the observed concentrations, the decision to consider alternate modeling techniques is clear, provided the emissions or meteorological data bases are not at fault. When the comparison shows that the model consistently overpredicts observed concentrations, the decision to recommend a different model may be considered.

Effective air quality decisions must be based on realistic modeling estimates. At times, selection of the most appropriate, realistic modeling technique is very difficult to make. Collection and use of high quality monitoring data are essential in evaluating decisions based on modeling data alone.

When are air quality data more acceptable than models in decision-making?

Air quality modeling is a tool used to estimate maximum expected pollutant concentrations over a wide range of meteorological conditions with the expectation that pollutant emission rates will at times reach their maximum allowed limits. Air quality data, on the other hand, represent pollutant concentrations measured when emission rates are at their actual levels. These rates could be below maximum allowed rates for much of the time. If modeling shows that no violation of the NAAQS is expected, but subsequent monitoring reveals excursions of the standards, then the air quality data take precedence over the modeling results.

Air quality data are also extremely important in situations where either the data base needed for modeling is inadequate, or the applicability of modeling in general is questionable. Model-based estimates of air quality and preliminary decisions may still be made, but these will usually be subject to review once additional monitoring data are obtained.

For More Information

Screening Procedures

Guidelines for Air Quality Maintenance Planning and Analysis, Vol. 10 (Revised), Procedures for Evaluating Air Quality Impact of New Stationary Sources. OAQPS No. 1.2-029R, EPA-450/4-77-001, October 1977.

Descriptions of Available Models

Guideline on Air Quality Models. OAQPS No. 1.2-080, EPA-450/2-78-027, April 1978.

Workbook for the Comparison of Air Quality Models. OAQPS No. 1.2-097, EPA-450/2-78-028A, May 1978.

Air Quality Monitoring Procedures

Ambient Air Monitoring Guidelines for PSD. OAQPS No. 1.2-096, EPA-450/2-78-019, May 1978.

U.S. Government Printing Office: 1980- 735-000/3017 Region No. 3-II

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